EFFECT OF NOTCH GEOMETRY ON MECHANICAL PROPERTIES OF PURE COPPER USING MD SIMULATION

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By

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CERTIFICATE

This is to certify that the thesis entitled "**EFFECT OF NOTCH GEOMETRY ON MECHANICAL PROPERTIES OF PURE COPPER USING MD SIMULATION"**, submitted to National Institute of Technology, Rourkela by **BibhudattaSahu(110MM0378)** in partial fulfillment of the requirements for the award of the degree of **BACHELOR OF TECHNOLOGY** in **Metallurgical and Materials Engineering** is an authentic work carried out by them under my supervision and guidance. The matter embodied in the thesis has not been submitted to any other University/ Institute for the award of any degree or diploma.

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ABSTRACT

The aim of this investigation is to study the effect of various notch geometries on the tensile and compressionbehaviors of nano-scalecopper at various temperatures through simulations based on molecular dynamics. In view of this, first simulation boxes have been created comprising of cylindrical, square and v-notches. Simulations for tensile and compression deformations have been done for all un-notched and notched specimens at different temperatures (viz. 100 K, 200 K, 300 K, 400 K and 500 K). The results indicate that yield and tensile strength values decreases with increase in temperature for all notched and un-notched simulation boxes. Strength values increase with introduction of notches of all geometries as compared to the un-notched ones, at all temperatures.In contrast to the tensile strength, it is found that the compression strength of notched specimen decreases with introduction of notches at a particular temperature.The variation in strength is attributed to the formation of stress triaxiality around the tip of the notch and plastic constraint factor. The square notch is the highest contributor to increase the tensile strength. Overall, it can be stated that molecular dynamic simulation can be effectively used to study the deformation behaviour of notched specimens.

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CHAPTER 1

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Background of Research

Objectives

Summary

1.1. Background of research :

It is known that before using a material for any engineering application,it needs to investigate the mechanical properties of the respective material which may include tensile and compression deformation behaviour, itsstiffness, ductility, hardness etc. Traditionally tensile behaviour of a ductilematerial is studied using a dog bone type of specimen as per ASTM standard E8M [1]. More precisely, it can be stated that the central part of thistype of a specimen is smooth. One can generally predict that the mechanical properties of a specimen may vary based on the conditions of the surface of the specimen. Ductility measurements on standard smooth tensile specimens donot always reveal metallurgical or environmental changes that lead to reduced local ductility[2]. On loading, the stress distribution of a specimen varies in case of presence of a discontinuity on the surface of it. This kind of stress distribution may be considered as triaxial state of stress. The tendency for reduced ductility in presence of a triaxial stress field and steep stress gradients is called notch sensitivity[2]. In practical situations,a component/material always have some irregularities like cracks, pores etc. on or beneath the surface. Therefore it is always needed to study the mechanical behaviour of the material when irregularities are present. This will help to predict the mechanical behaviour in actual service condition.

There are different types of notches used during during a simulation. Different types of notch geometry can alter the mechanicalbehaviour to the specimen. But in lab experiment we generally use V-notched specimen. But in actual practice notch may be of different geometry like angular, square, cylindrical, spherical, conical etc. There are irregularities present in different types of notch geometries.

Computer based molecular dynamics (MD) simulation is now-a-days potentially utilized to determine different material behaviours. Computer simulations act as a channel between microscopic length and time scales and the macroscopic world of the laboratory[3]. It provides information related to the interactions between atoms, and exactly predicts the mechanical properties. The predictions& observation can be made as precise and accurate as we like, subject to the limitations imposed by our computer’s ability.Using molecular dynamics (MD)

simulation, fracture mechanisms of nanoscale pure iron under static and symmetric cyclic loading conditions have been performed by Inoue et al [4].Li and his co-workers investigated the cyclic stress/strain evolutions for tensile strengthprediction through simulation studies; it was found that the determination of tensile strength depends not only on the specimen models, but also on the accurate evaluations of the cyclic elasto-plastic stress/strain responses [5]. The tensile and compression behaviour of nano-scale copper with vacancies at various temperatures has been studied using MD simulation by Chang[6]. Chang and Fang investigated the influence of tensile and compression behaviour of nanoscale copper through MD simulation. Themechanical properties of nano-structured copper have been of significant interest to researcherssince the development of electronic industry. Most of the existing investigations are based on experimental results and findings. Reports are also available based on simulation of tensile and compression behaviour through simulated models. As molecular dynamics (MD) simulation encounters studying the behaviour of 99.9999% pure material, in this investigation tensile and compression behaviour of pure copper is studied to understand the effects of notch geometry in it.

1.2. Objectives

The main objectives to fulfil these can be broadly summarized as:

(I) To find tensile and compression behaviour of nano-scale copper at different temperatures:-

This part consists of

(a) Generating plots for tensile stress vs. strain curves of nano-scale copper at different temperatures for both notched & un-notched specimen.

(b) Study variation in the tensile and compression strength, yield strength of nano-scale copper at different temperatures.

(c)Study variation in % total elongation & % uniform elongation at variation of temperature.

(2)To find tensile and compression behaviour of nano-scale copper at different notch geometries:-

This part consists of

(a) Generating plots for tensile stress vs. strain curves of nanoscale copper at different notch geometries.

(b) Study variation in the tensile and compressive strength of nanoscale copper at different notch geometries at a particular temperature.

1.3. Summary:

The thesis has been Subdivided into five chapters. There is briefing of the significance of the problem and relates research behind this investigation in **Chapter-1**. Some relevant literature background related to the current investigation of tensile &compressionbehaviour and molecular dynamics simulation has been presented in **Chapter-2**. **Chapter-3** consists of simulation parameters to perform simulation studies on nano-scale copper along with the description of the simulation procedure regarding tensile & compression behaviour behind these simulations. **Chapter-4** consists the results and discussion related to the above stated objectives. **Chapter-5** is an overview of the conclusions derived from this study which has been analysed briefly with few directions for future work related to this section. A comparison has also been made with the results obtained from this investigation with those of previous investigations. All references cited throughout the work have been compiled at the end of **Chapter-5**.

Literature Survey

CHAPTER 2

OUTLINE

Introduction

Parameters related to stress vs strain curve

Notch effects

Some previous investigation related to this study

Molecular dynamics simulation

Advantages of using molecular dynamics simulation

Review of the current problems

2 .1 INTRODUCTION :

The stress-strain curve's magnitude and shape depends upon its composition, heat treatment and temperature, strain rate, etc.

2.1.1 PARAMETERS RELATED TO STRESS VS STRAIN CURVE:

TENSILE STRENGTH

The tensile strength or ultimate tensile strength(UTS) is the maximum load divided by the cross sectional area of the specimen.

$$Su = Pmax / Ao$$

The tension test calculates the values of UTS.For ductile material UTS is defined as the measure of the maximum load which a metal can withstand under very restrictive condition of uniaxial loading.For several years it served to define the strength of materials or tensile strength. But nowadays it is used in basing the static design of ductile metalson the yield strength.Moreover because of long duration of using tensile strength to calculate the strength of the materials, it has become a familiar property and identification of the materials.

MEASURE OF YIELDING

The stress at which plastic deformation or yielding is observed depends on the sensitivity of strain measurements. Most materials gradually change from elastic to plastic behaviour, the particular point at which plastic deformation begins is difficult to determine. Various criteria for the initiation of yielding depends on the sensitivity of the strain measurements. Fig-2.1 gives the basic idea of stress vs strain curve [2]

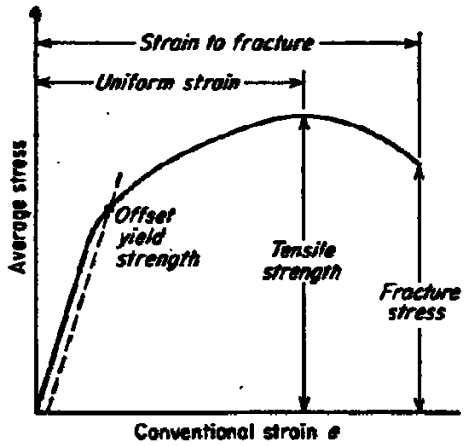


Fig-2.1 Stress vs strain curve

Elastic limit is the maximum stress the material can withstand without any measurable strain remaining on the complete release of load. By increasing the sensitivity of strain measurement, the elastic limit is reduced until it equals to true elastic limit. Elastic limit determination requires too long loading-unloading test procedure. The yield strength is the stress required to produce a small amount of plastic deformation.

So=P (strain offset=0.002)/Ao

From the stress-strain curve we can determine the % uniform elongation & % total elongation.% uniform elongation is the point at the UTS at which necking starts. Up to this point the elongation will be uniform. After necking there come voids in the specimen. So the elongation will not be uniform anymore. At the fracture point the total strain will be % total elongation.

MODULUS OF ELASTICITY

It is the slope of the linear portion of the stress-strain curve. It measures stiffness of the material. The binding force of the atoms determines the MODULUS OF ELASTICITY . These forces can't be altered without changing the nature of material. So it is the most structure insensitive property of the material. With increasing temperature the UTS and hence the Young's modulus of the material diminishes.

2.1.2 NOTCH EFFECTS :

The changes produced by the notch geometries have important ramifications in fracture process. Introduction of notch creates a local stress peak at the root of the notch.Plastic flow begins here when local stress reaches yield strength of the material.It limits the peak stress to yield stress of the material.The main effect of the notch is to create stress tri-axiality at the notch.

The elastic stress distribution in a notched thin plate is shown in fig 2.2.1. In this case two directional stresses are developed at the notch. Transeverse elastic stress σ_x & longitudinal stress σ_y is generated. But for thick specimen as fig 2.2.2. three components of stresses are generated at the notch tip. The distribution of σ_z with z at the notch root (x=0) is shown in fig-2.2.3. The values of σ_y &σ_x are nearly independent of z. Fig 2.2.2 shows that stressing a thick specimen provides stress triaxiality at the notch tip. As a consequence of stress triaxiality at the notch the yield stress will be more as compared to uniaxial yield stress because it is more difficult to spread yielded zone in case of stress triaxiality. The ratio of notched to unnotched flow stress is called plastic constraint factor. Orowan has shown this value cannot exceed 2.57. Thus this triaxial stress of a notch results in notch strengthening in a ductile metal but in case of brittle material this value exceed before the material undergoes plastic yielding.[2]

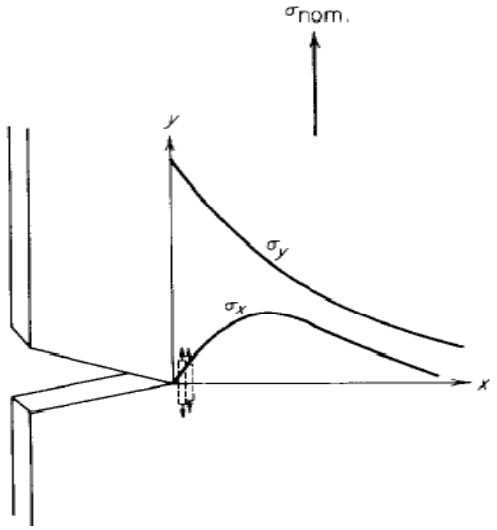


Fig.-2.2.1 Elastic stresses under a notch in a thin plate[2]

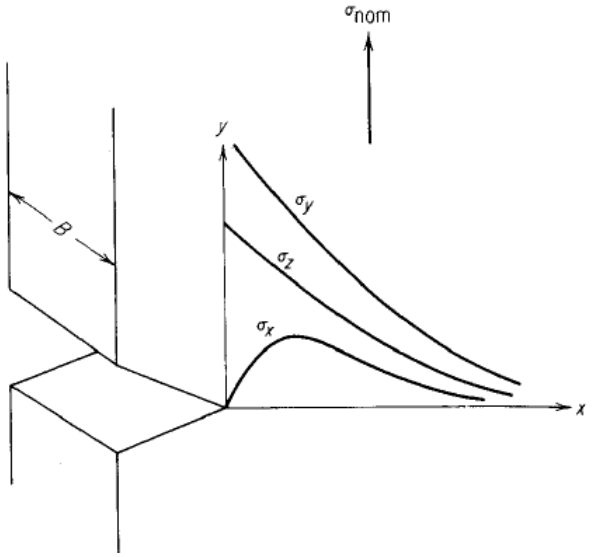


Fig.-2.2.2 Elastic stresses under a notch in a thick plate[2]

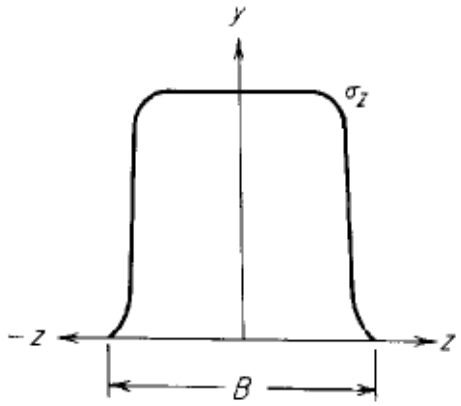


Fig-2.2.3 Distribution of σ_z with z at x=0[2]

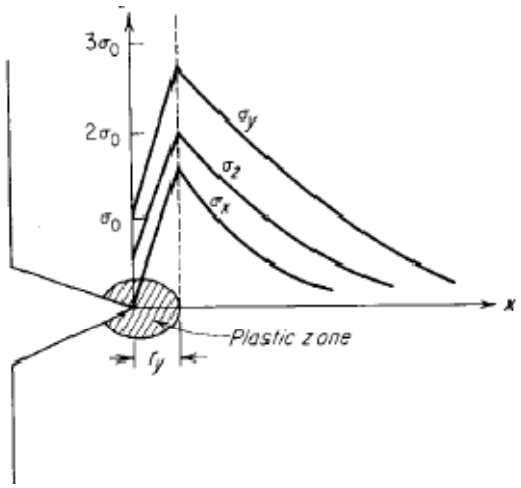


Fig-2.2.4 Distribution of stresses during local yielding[2]

The tendency for reduced ductility in presence of a triaxial stress field is called notch sensitivity. Notch introduction creates plastic constraint factor. Because of this plastic constraint factor tensile strength will be more than an unnotched specimen. The common way to detect notch brittleness or high notch sensitivity is by calculating notch strength ratio (NSR).

NSR=Snet/Su

Snet is used for notched specimen & Su is used fortensile strength for unnotched specimen

If NSR<1, then material is notch brittle. There is also reduction of area at the notch.

2.2 SOME PREVIOUS INVESTIGATION RELATED TO THIS STUDY :

Since few years, the study of the mechanical properties of nanostructured materials usingatomistic simulation has been of prime interest to researchers due to nano-technological development [7–9]. For example, Miyazaki and Shiozaki [10] calculated the elastic constant and thermal expansion coefficient of Fe. Aya and Nakayama [11] investigated the influence of environmental temperature on the yield stress of polymers. The material stiffness is one of the significant properties of a material. Miller and Shenoy [12] studied the bending stiffness properties of nanosized structural Al and Si. Since the rebirth of the electronic industry, copper has been one of the important materials in the field [13]. Many have studied the material

properties of copper. Heino et al. [14] investigated the mechanical properties of copper, including the elastic constant and the demeanour of crack propagation at room temperature.Schiotz et al. [15] studied the effects of strain rate and porosity on the mechanical deformation of copper at several temperatures. Recently, Kang and Hwang [16] investigated mechanical deformations of copper nanowire.

Earlier scientists have studied about the behaviour of nano-scale copper using MD simulation. But Chang has studied the mechanical behaviour of nano-scale copper where vacancies are present inside the box using MD simulation as fig-2.2. The behaviour will change as compared to the normal box dimension.

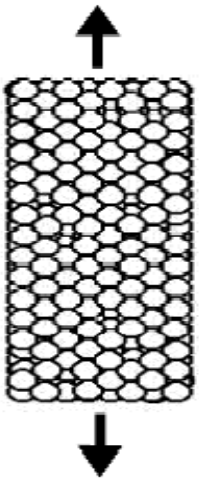


Fig-2.3 Configuration of nano-scale copper with vacancies for the tensile test[6]

He has studied the tensile behaviour for various amount of vacancies at a particular temperature and the effect of tensile behaviour on temperature as shown in fig-2.3, 2.4. From the observation he concluded that with increase in vacancies of nano-scale copper the UTS reduces considerably. He also concluded that the UTS of nano-scale copper decreases with rise in temperature. His investigation may help us for our study related to tensile & compression behaviour of nano-scale copper using MD simulation.

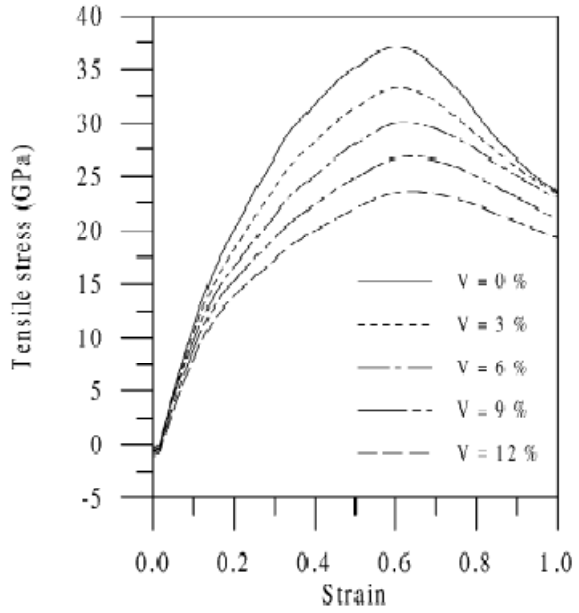


Fig. 2.4 Relationship between tensile stress and strain for nanoscale copper with various vacancies at T5300 K.[6]

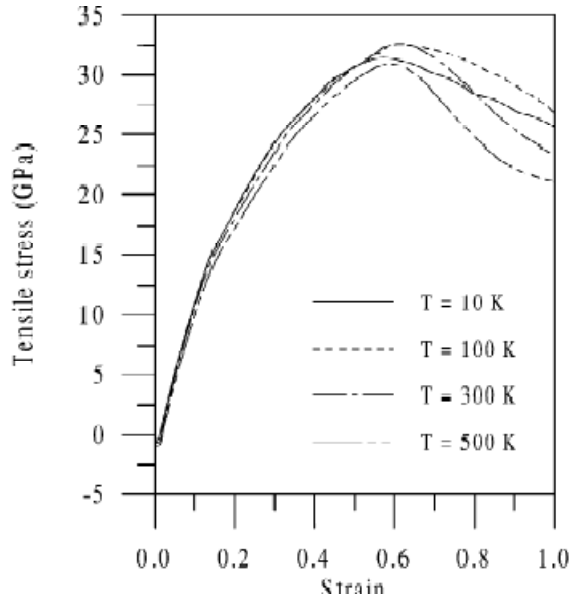


Fig. 2.5. Relationship between tensile stress and strain for nanoscale copper with V56% at various temperatures.[6]

2.3Molecular dynamics simulation :

Molecular dynamics (MD) simulation is a computer based simulation of the movements of atoms and molecules.In this process, the molecules are allowed to interact with each other for a certain periodof time. Normally, the paths of atoms and molecules are decided by solving the Newton's equations of motion for a system of interacting particles, where forces among particles are defined by force fields of molecular mechanics. These simulations can be used to find macroscopic thermodynamic properties of the system. MD simulation is also called as statistical mechanicsby numbers" and "Laplace's vision of Newtonian mechanics" as it foretells the future by emanatingthe forces of nature and providing a view into motion of molecules on an atomic scale. A molecular dynamics simulation requires a description of the particles in the simulationwhich will interact. The upper hand using MD is that it gives an idea of dynamical properties of the system: transport coefficients, time-dependent responses to changes, rheological properties and spectra. Potentials is known at many levels of physical accuracy; those mostcommonly used in chemistry are based on molecular mechanics and indivisualise a classicaltreatment of particle-particle interactions that can generate structural and conformational changesbut usually cannot generate chemical reactions.

2.4 Advantages of using Molecular Dynamics Simulation:

- For the investigators conducting tensile & compression tests at high temperature really a challenge and needs long duration of time. Hence manymolecular simulation studies have come into a scenario to predict the tensile and compression behaviour of materials at changing temperatures.
- Using molecular dynamics simulation, 100% pure copper can beobtained which is practically a Herculean task.
- However, testing can be carried out at low temperature,room temperature and elevated temperatures at the same time, facilities for which are unavailable in ourlaboratories.
- To create perfect notch of different geometries practically is hard & time consuming. Using MD simulation we can avoid these restrictions.

In this report an attempt has been made to gain some knowledge on tensile &compression behaviour of materials via MD simulations.

2.5 Review of the current problem :

There are numerous investigations related to tensile &compression behaviour of materials under different temperature & stress applied.

Most of these investigations mostly verify the effect of temperature on the tensile & compression property of nano-scale copper and how the presence of different types of notch geometry differs from the un -notched condition.

This investigation, in brief, attempts to understand:

(i) Tensile behaviour of the investigated material i.e. nano-scale copper at various temperatures and different types of notch geometry.

(ii) The % elongation & tensile strength at various temperatures and notch geometry in nano-scale copper.

Molecular Dynamics Simulation using LAMMPS

CHAPTER

OUTLINE

Introduction

Simulation Procedure

Simulation Parameters

Sample Configuration

Input file of un-notched specimen

Tensile Test

(a)Input file for tensile testing

(b)ductile fracture through tensile simulation

Compression test

Input file for compression testing

Brittle fracture through compression simulation

3 MOLECULAR DYNAMICS(MD) SIMULATION USING LAMMPS

3.1 INTRODUCTION :

In this experiment, Molecular Dynamics(MD) simulation of nano-scale copper has been verified using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). LAMMPS is a molecular dynamics simulation code designed to run effectively on parallel computers. It is an open-source code that models acluster of particles in all material states. It can model atomic, polymeric, metallic, granular, and coarse-grained systems by a varied force fields and boundary conditions.

LAMMPS integrates Newton's equations of motion for collections of molecules, atoms, or macroscopic particles which interact by short- or long-range forces with a varianceof boundary conditions. For computational efficiency, LAMMPS uses neighbouring liststo follow up nearby particles. On parallelmachines, to devide the simulation domain into small 3d sub-domains, LAMMPS uses special decomposition techniques.

A LAMMPS input script has 4 parts:

1. Initialization
2. Atom definition
3. Settings
4. Run a simulation

LAMMPS executes commands from an input script (text file), reading one row at a time. It exits when the input script finishes. Every command results LAMMPS to perform an activity; it can read in a file, set an internal variable, or run a simulation. Normally, the ordering of commands in an input script is of less importance.

However the following points should be looked upon:

(1) LAMMPS reads the input script line by line and each command takes effect
As soon as when it is read, not after the entire text file is read.

(2) A few commands are valid only when they follow other commands. A group
Command can only be used after the atoms are defined.

(3) Sometimes a command X may use values set by command Y. This means command X must follow command Y in the input script if it is to have the required effect.

3.2 Simulation procedure

.

In our simulations we used EAM FS (Finnis-Sinclair) potential developed by Mendelev et al [23] and it is a valid potential. In the EAM, the total energy of an *N*- atom system is represented in the following equation:

, ,

$$E_{\text{tot}} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{\substack{i,\ j \\ i \neq j}} \varphi_{i,\ j}(r_{i,\ j})$$

where$\varphi_{i,j}(r_{i,j})$is a short range pair potential between atom *I* and *j* with the separation distance $_{i\ j}\ r\ ,\ ,\ (\ )\ _{ii}F\rho$ is the embedding energy of atom *I* with the electron density $_i\rho$ due to all its neighbors is expressed below:

$$\rho_i = \sum_{j \neq i} f_j(r_{i\ j})$$

In Finnis/Sinclair model the total energy of an atom is represented by the following equation:

$$E_i = F_\alpha\left(\sum_{j \neq i} \rho_{\alpha,\beta}(r_{i,j})\right) + \frac{1}{2}\sum_{j \neq i} \varphi_{\alpha,\beta}(r_{i,j})$$

whereρ the electron density is a functional specific to the atomic types of both atoms *I* and *j* so that different elements can attribute variedly to the total electron density at an atomic site depending on the identity of the element at that atomic site and alpha and beta are the element types of atom *I* and *j*. The initial amorphous structures for simulation were obtained using NPT

ensemble with zero applied pressure. Timestep is equal to 0.002 ps. Equations of motion are numerically integrated using velocity-Verlet algorithm.

3.3. Simulation Parameters:

LAMMPS requires as input a list of initial atom coordinates and types, molecular topology information, and force-field coefficients given to all atoms and bonds.It has potentials for soft materials viz. biomolecules, polymers; solid-state materials viz. metals, semiconductors and coarse-grained or mesoscopicsystems.VMD is a simple and fast visualizer provided with the LAMMPS package which creates xyz projection views of atomic coordinates and animates them. Through VMD we can prognosticates the differences happening step by step in the simulation.

At the time of writing the simulation input file code, variables like potential file, lattice parameters, maximum and minimum stress, temperature, number of cycles and number of iterations are altered. These parameters control the simulation conditions and environment. For atomic systems LAMMPS provides a create atoms command which puts atoms on solid-state lattices(fcc, bcc, user-defined, etc). Ascribing less numbers of force field coefficients can be done through the pair coeff, bond coeff, angle coeff, etc commands.

Simulation box size, time step and total time frame must be adjusted such that the calculation can end within a reasonable time period. Moreover, the simulations should be made as long as it can be so as to coincide the time scales of the natural processes being studied, i.e. to make statistically valid conclusions, the time frame of the simulation should coincide the kinetics of the natural process. The timestep should be small enough so as to prevent discretization errors.The simulation box size must be large enough to prevent boundary condition artifacts. Boundary conditions are often treated by selecting fixed values at the edges or by deploying periodic boundary conditions in which one side of the simulation loops back to the other side,imitating a bulk phase.

NVE (Micro-canonical ensemble): In NVE ensemble, the system undergoes an adiabatic process and is isolated from changes in moles (N), volume (V) and energy (E).

NVT (Canonical ensemble): In NVT, also sometimes called as constant temperature molecular dynamics (CTMD), moles (N), volume (V) and temperature (T) are conserved and the energy of endothermic and exothermic processes is exchanged with a thermostat.

NPT (Isothermal–isobaric) ensemble: In NPT ensemble, moles (N), pressure (P) and temperature (T) are conserved. A barostat is also needed along with a thermostat. It corresponds to laboratory conditions with a flask open to ambient temperature and pressure

3.4. Sample Configuration:

The initial configuration of four different samples for various molecular dynamics simulations isshown in Fig. 1,Fig. 2, Fig.3 & Fig. 4. Both tensile and compression simulations were performed using this type of sampleconfiguration. The assembly contains three regions; grip region at the opposite ends which iscomposed of immobile atoms and tension/tension-compression region which include the mobileatoms. Tensile and Compression loading were carried out in the both x,y-direction, as indicated inFig. 3.1. The periodic boundary condition was imposed on the x and z axis and the material wasfree to be strained in the y-direction only.

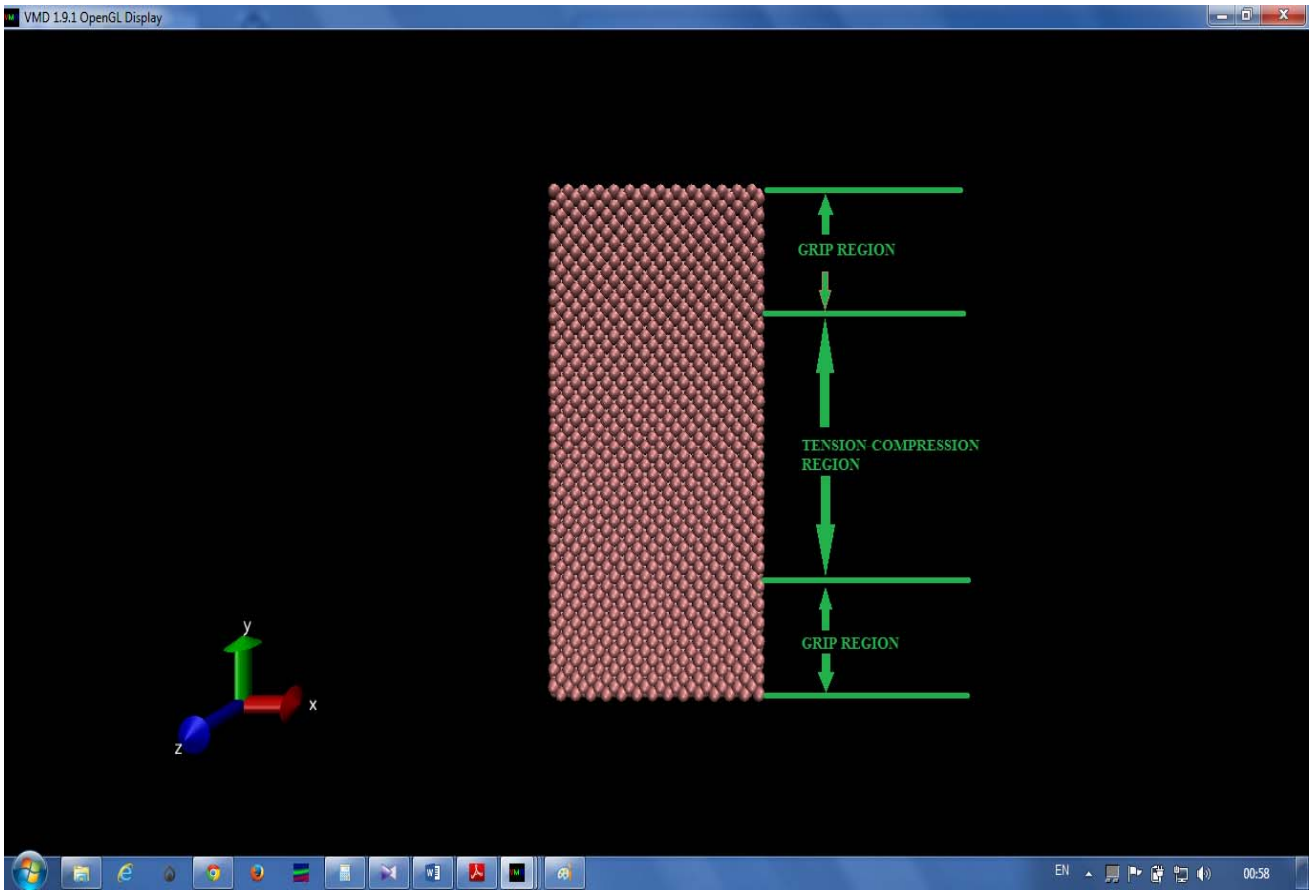
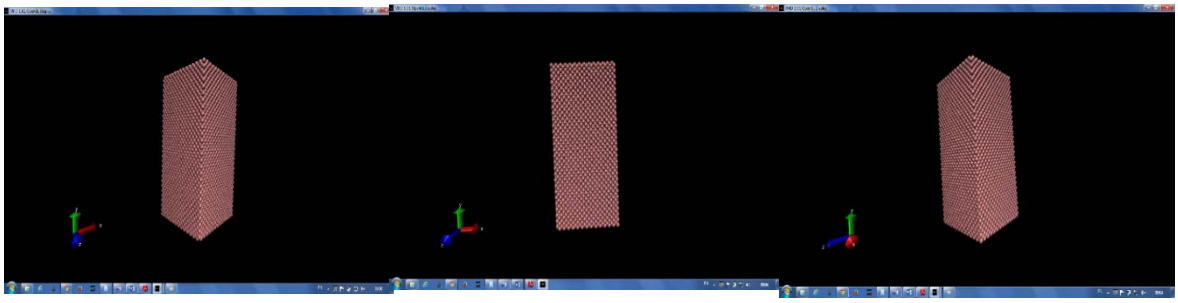
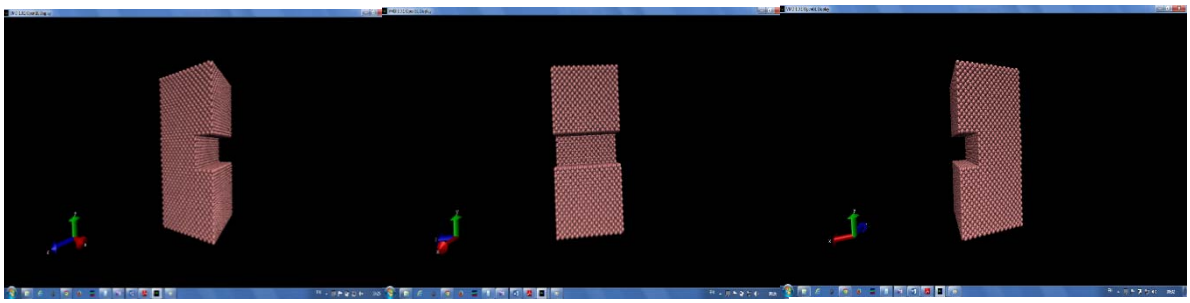


Fig.3.4.1: VMD snapshot of the Cu sample undergoing simulation.



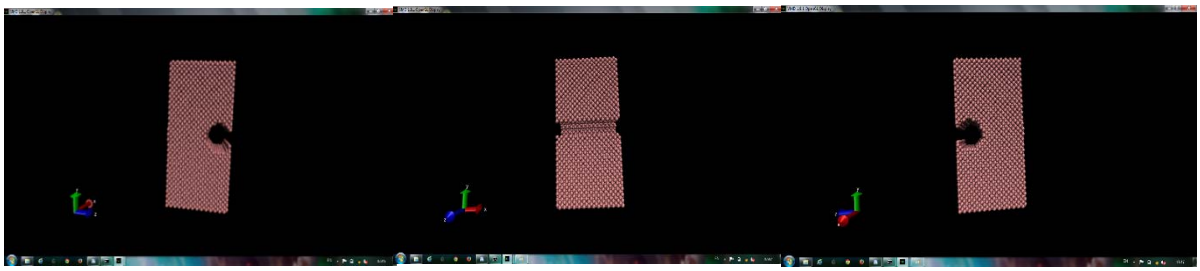
(left side view) (front view) (right side view)

Fig. 3.4.2 Different sectional view of Un-notched Sample:



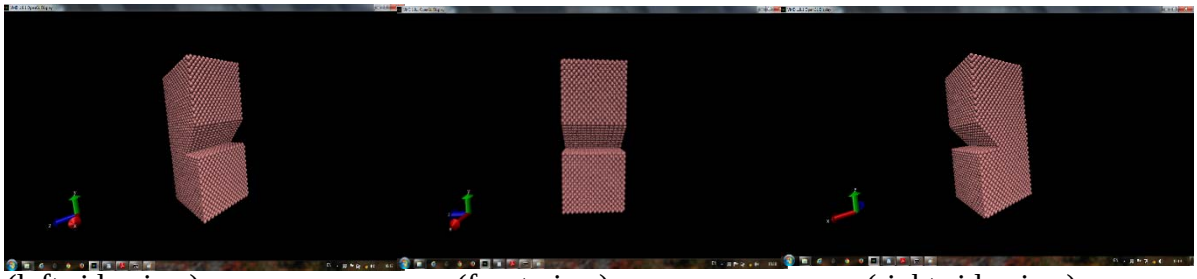
(left side view) (front view) (right side view)

Fig. 3.4.3 Different sectional view of square-notched Sample:



(left side view) (front view) (right side view)

Fig. 3.4.4 Different sectional view of cylindrical-notched Sample:



(left side view) (front view) (right side view)

Fig. 3.4.5 Different sectional view of V-notched Sample:

SI. No.	Sample type	Box Dimension	Total number of Atoms
1.	Un-Notched	50 x 100 x 50	21952
2.	Square-Notched	50 x 100 x 50	20720
3.	Cylinder-Notched	50 x 100 x 50	20602
4.	V-Notched	50 x 100 x 50	21182

Table 3.4.1: Size and Dimensions of Sample with different notch geometry Undergoing Simulation

3.4.1. Input file for obtaining equilibrated 3D-crystal lattice of Un-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **…→specifies units of every quantity used in the input file**

echoboth**…→reverberates each input script command to log file and screen**

atom_style atomic

dimension 3

boundary p pp**…→periodic boundary condition**

region box block 0 50 0 100 0 50 units box **→specifies a geometric region of space**

create_box 1 box**.....→generates a simulation box in the defined region**

lattice fcc 3.61**……..→lattice type and lattice parameter**

region cu block 0 50 0 100 0 50 units box

create_atoms 1 region cu units box**…→ generates copper atoms in the simulation box**

timestep 0.002**……→ sets the timestep for subsequent simulations**

pair_styleeam/alloy

pair_coeff * * Cu_zhou.eam.alloy Cu**……→defines the potential file used**

 # Energy Minimization

#minimize 1.0e-7 1.0e-8 1000 1000

thermo 100**→computes and prints thermodynamic**

thermo_style custom step temp vol press etotal**→ defines content of thermodynamic data to be printed in screen &**

computemyRDF all rdf 1000

fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj

..…→dumps a snapshot of atom quantities every 10 time steps to the specified file

dump_modify 1 scale no**…→changes parameters of prior specified dump command.**

A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… →closes the current log file, opens a new log file, and begins logging information to it

velocity all create 300 873847 rot yes mom yes distGaussian**…→assigns the velocity of a group of atoms**

#fixes

fix 1 all npt temp 100 100 0.1 iso 0 0 0.1→**temp and pressure preserved**

run 1000**… → program is run for 1000 iterations**

unfix 1 **… →omits the previously defined fix 1**

3.4.2. Input file for obtaining equilibrated 3D-crystal lattice of Square-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **…→defines units of all quantities used in the input file**

echoboth**…→reverbates each input script command to log file and screen**

atom_style atomic

dimension 3

boundary p pp**…→periodic boundary condition**

region box block 0 50 0 100 0 50 units box →**specifies a geometric region of space**

create_box 1 box**.....→gnerates a simulation box in the defined region**

lattice fcc 3.61**……..→lattice type and lattice parameter**

region cu block 0 50 0 100 0 50 units box

create_atoms 1 region cu units box**…→ generates copper atoms in the simulation box**

region cu1 block 35 50 40 60 0 50 units box→**defines a geometric region of Square-notch**

group crystal region cu1

delete_atoms group crystal**…→generates square-notch in the simulation box**

timestep 0.002**……→assigns the timestep for subsequent simulations**

pair_styleeam/alloy

pair_coeff * * Cu_zhou.eam.alloy Cu**……→defines the potential file used**

 # Energy Minimization

#minimize 1.0e-7 1.0e-8 1000 1000

thermo 100→**computes and prints thermodynamic**

thermo_style custom step temp vol press etotal→ **specifies content of thermodynamic data to be printed in screen &**

computemyRDF all rdf 1000

fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj

..…→dumps a snapshot of atom quantities every 10 time steps to the specified file

dump_modify 1 scale no**…→alters parameters of prior defined dump command.**

A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… →closes the current log file, opens a new log file, and begins logging information to it

velocity all create 300 873847 rot yes mom yes distGaussian**…→sets the velocity of a group of atoms**

#fixes

fix 1 all npt temp 100 100 0.1 iso 0 0 0.1**→temp and pressure conserved**

run 1000**… → program is run for 1000 iterations**

unfix 1 **… →omits the previously defined fix 1**

3.4.3. Input file for obtaining equilibrated 3D-crystal lattice of Cylinder-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **…→defines units of all quantities used in the input file**
echoboth**…→reserverates each input script command to log file and screen**
atom_style atomic
dimension 3
boundary p pp**…→periodic boundary condition**
region box block 0 50 0 100 0 50 units box **→defines a geometric region of space**
create_box 1 box**.....→generates a simulation box in the specified region**

lattice fcc 3.61**……..→lattice type and lattice parameter**
regioncu block 0 50 0 100 0 50 units box
create_atoms1 region cu units box**…→ creates copper atoms in the simulation box**

region cu1 cylinder x 50 40 10 0 50 units box→**defines a geometric region of Cylinder-notch**

group crystal region cu1

delete_atoms group crystal**…→ creates square-notch in the simulation box**

timestep 0.002**……→ assigns the timestep for subsequent simulations**

pair_styleeam/alloy

pair_coeff * * Cu_zhou.eam.alloy Cu**……→specifies the potential file used**

 # Energy Minimization

#minimize 1.0e-7 1.0e-8 1000 1000

thermo 100→**computes and prints thermodynamic**

thermo_style custom step temp vol press etotal→ **specifies content of thermodynamic data to be printed in screen &**

computemyRDF all rdf 1000

fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj

..…→dumps a snapshot of atom quantities every 10 time steps to the specified file

dump_modify 1 scale no**…→alters parameters of prior defined dump command.**

A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… →closes the current log file, opens a new log file, and begins logging information to it

velocity all create 300 873847 rot yes mom yes distGaussian**…→sets the velocity of a group of atoms**

#fixes

fix 1 all npt temp 100 100 0.1 iso 0 0 0.1**→temp and pressure conserved**

run 1000**… → program is run for 1000 iterations**

unfix 1 **… →omits the previously defined fix 1**

3.4.4. Input file for obtaining equilibrated 3D-crystal lattice of V-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **…→ defines units of all quantities used in the input file**

echoboth**…→reserverates each input script command to log file and screen**

atom_style atomic

dimension 3

boundary p pp**…→periodic boundary condition**

region box block 0 50 0 100 0 50 units box **→defines a geometric region of space**

create_box 1 box**.....→generates a simulation box in the specified region**

lattice fcc 3.61**……..→lattice type and lattice parameter**

region cu block 0 50 0 100 0 50 units box

create_atoms 1 region cu units box**…→ creates copper atoms in the simulation box**

regioncu1 prism 30 50 40 60 0 50 20 0 0 units box→**defines a geometric region of V-notch**
group crystal region cu1
delete_atoms group crystal**…→ creates square-notch in the simulation box**

timestep 0.002**……→ sets the timestep for subsequent simulations**
pair_styleeam/alloy
pair_coeff * * Cu_zhou.eam.alloy Cu**……→specifies the potential file used**

 # Energy Minimization
#minimize 1.0e-7 1.0e-8 1000 1000

thermo 100→**computes and prints thermodynamic**
thermo_style custom step temp vol press etotal→**specifies content of thermodynamic**
data to be printed in screen &

computemyRDF all rdf 1000
fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj
..…→dumps a snapshot of atom quantities every 10 time steps
to the specified file
dump_modify 1 scale no**…→modifies parameters of previously defined dump command.**
A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… →closes the current log file, opens a new log file, and begins logging information to it

velocity all create 300 873847 rot yes mom yes distGaussian**…→sets the velocity of a group of atoms**

#fixes

fix 1 all npt temp 100 100 0.1 iso 0 0 0.1**→temp and pressure conserved**

run 1000**… → program is run for 1000 iterations**

unfix 1 **… →deletes the previously defined fix 1**

3.5. Tensile Test:

It is expected for any MD simulation study that an energy minimization of the system is required before performing the actual simulation studies. Through repeated adjustment of atom coordinates, the configuration attains a position of minimum local potential energy. The configuration used for tensile testing was therefore caliberated at room temperature using the method specified above. The tensile test was then carried out at five different temperatures viz. 100 K, 200 K, 300K, 400K and 500 K with the parameters as mentioned in Table 1. The strain in the y direction was calculated using the following equation:

$$e = \text{loading rate} * \text{time} \qquad (3.4)$$

Where time = time step * step number (time step = 0.001 ps)
Loading rate = 0.1/ps

To understand the effect of notch geometry, simulations were carried out with similar box dimensions
[Table 1] and the typical outcome obtained was plotted in the form of stress-strain curves.

3.5.1. Input file for tensile testing of a previously equilibrated crystal:

 # 3d tensile simulation JP4review

```
units           metal
boundary        p pp
atom_style      atomic
echo        both
read_data       Test.dat→ reads the data file consisting the atom positions of the equilibrated crystal in the defined file

timestep    0.001

pair_style    eam/alloy
pair_coeff          * * Cu_zhou.eam.alloy Cu

# Energy Minimization
#minimize           1.0e-5 1.0e-10 10000 100000

dump            1 all atom 100 dump.Test_40%strain.lammpstrj
```

log log5050_Test_40%strain.dat

initial velocities

velocity all create 300 482748 rot yes mom yes distgaussian

fix 1 all deform 1 y erate 1.0**….→strain rate of 0.1 sec^{-1} is applied in y direction**

fix 2 all npt temp 100.0 100.0 10.0 x 0 0 10.0 z 0 0 10.0 dilate all**…→all atoms rescaled**

to new positions while temp and pressure is conserved

fix 3 all temp/rescale 10 100 100 0.05 1.0**→Resets the temp of atoms to 100K by rescaling velocities after every 10 steps**

compute 11 all rdf 100

fix 4 all ave/time 100 1 100 c_11 file rdf_Test_40%strain.rdf mode vector

compute 1 all stress/atom **…→ computes the symmetric per-atom stress tensor for each**

atom in a group.

compute 2 all temp**… → computes the temp of a group of atoms**

dump 2 all custom 1000 dump.stress_atom_Test_40%strain type x y z c_1[1] c_1[2] c_1[3] c_1[4] c_1[5] c_1[6]**→dumps atom type; x,y,z coordinates; 6 stress tensors computed in 1 to an array of 6 elements**

compute 3 all reduce sum c_1[2]→**decreases vector quantities of every stress tensor in y-direction and adds all the quantities to a single**

variable stress equal c_3/(3*40000)→**prescribes a value to the variable name stress**

variablestress_GPa equal v_stress/10000→**changes the stress determined to GPa**

variablestress_MPa equal v_stress_GPa*10000

variable tmp equal ly

variable lo equal ${tmp}

variable strain equal (ly-v_lo)/v_lo

variable p equal -pyy/10000→**prescribe a value to the variable name strain**

thermo 10

thermo_style custom step temp press voletotal c_2 v_stressv_stress_GPav_stress_MPav_strain

run 4000**…** → **number of iterations is given so as to give 40% strain to the material**

3.5.2.The Ductile fracture in Nanoscale Copper through Tensile Simulation code

Fig-3.5.1 VMD snapshot of Tensile testing of unnotched specimen during simulation

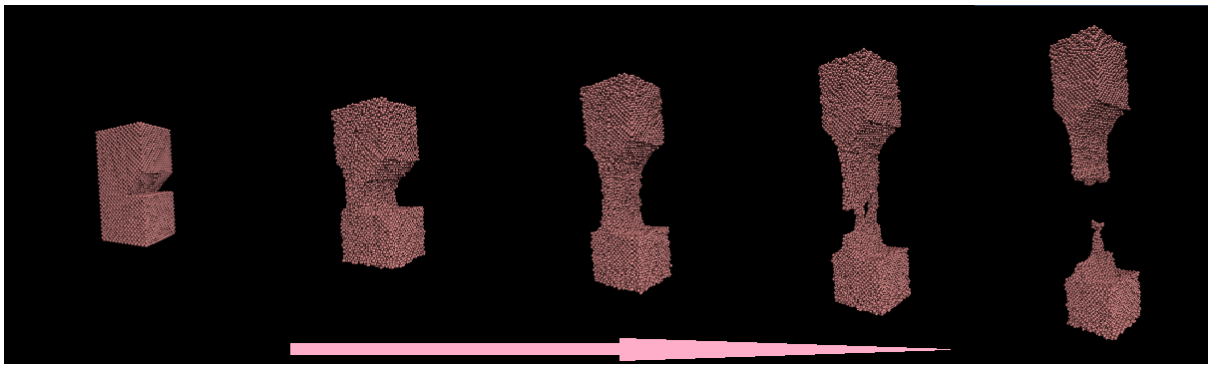


Fig-3.5.2 VMD snapshot of Tensile testing of V-notched specimen during simulation

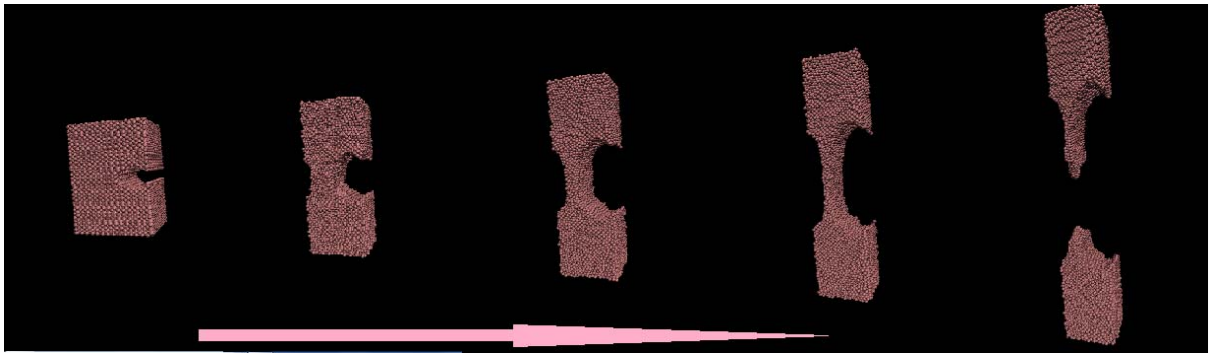


Fig-3.5.3 VMD snapshot of Tensile testing of cylindrical notched specimen during simulation

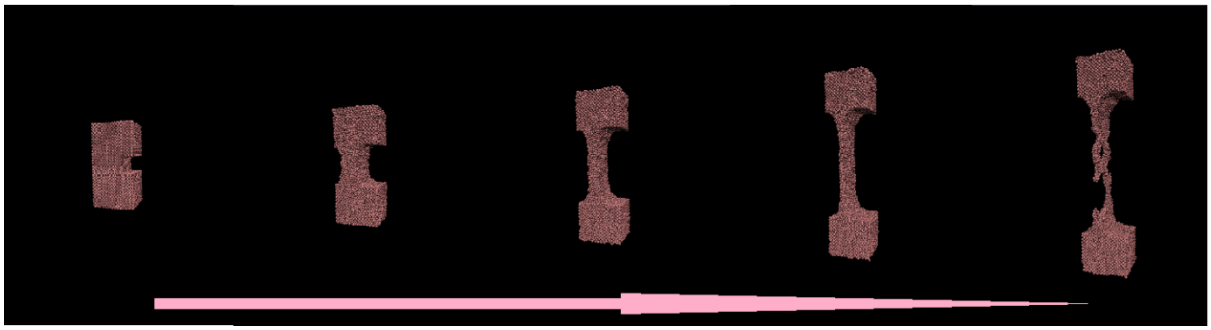


Fig-3.5.4 VMD snapshot of Tensile testing of square notched specimen during simulation

3.6. Compression Test:

In this experiment we also test the hardness of the materials at -0.1 strain rate with similar temperature (i.e. Room temperature) . Unlike the tensile testing here we get deformation of the Copper at a very low strain rate. The codes for compression in MD Simulations is same as Tensile simulation but here only the strain rate is negative and run time is much smaller in compare to tensile simulation.

3.6.1. Input file for compression testing of equilibrated crystal:

 # 3d compression simulation JP4review

```
units           metal
boundary        p pp
atom_style      atomic
echo        both
```

read_dataTest.dat→**reads the data file containing the atom positions of the equilibrated crystal in the specified file**

```
timestep    0.001

pair_style    eam/alloy
pair_coeff          * * Cu_zhou.eam.alloy Cu

# Energy Minimization
```

#minimize 1.0e-5 1.0e-10 10000 100000

dump 1 all atom 100 dump.Test_40%strain.lammpstrj
log log5050_Test_40%strain.dat

initial velocities

velocity all create 300 482748 rot yes mom yes distgaussian

fix 1 all deform 1 y erate-1.0**….→strain rate of -0.1 sec^{-1} is applied in y direction**
fix 2 all npt temp 100.0 100.0 10.0 x 0 0 10.0 z 0 0 10.0 dilate all**…→all atoms rescaled**
to new positions while temp and pressure is conserved

fix 3 all temp/rescale 10 100 100 0.05 1.0**→Resets the temp of atoms to 100K by rescaling velocities after every 10 steps**

compute 11 all rdf 100
fix 4 all ave/time 100 1 100 c_11 file rdf_Test_40%strain.rdf mode vector

compute 1 all stress/atom **…→ computes the symmetric per-atom stress tensor for each**
atom in a group.
compute 2 all temp**… → computes the temp of a group of atoms**

dump 2 all custom 1000 dump.stress_atom_Test_40%strain type x y z c_1[1] c_1[2] c_1[3] c_1[4] c_1[5] c_1[6]→**dumps atom type; x,y,z coordinates; 6 stress tensors computed in 1 to an array of 6 elements**

compute 3 all reduce sum c_1[2]→**reduces vector quantities of all stress tensors in y-direction and adds all the quantities to a single**

variable stress equal c_3/(3*40000)→**assigns a value to the variable name stress**

variablestress_GPa equal v_stress/10000→**converts the stress calculated to GPa**

variablestress_MPa equal v_stress_GPa*10000

variable tmp equal ly

variable lo equal ${tmp}

variable strain equal (ly-v_lo)/v_lo

variable p equal -pyy/10000→**assign a value to the variable name strain**

thermo 10

thermo_style custom step temp press voletotal c_2 v_stressv_stress_GPav_stress_MPav_strain

run 4000**…** → **number of iterations is given so as to give 40% strain to the material**

3.6.2.The Brittle fracture in Nanoscale Copper through Compression Simulation code

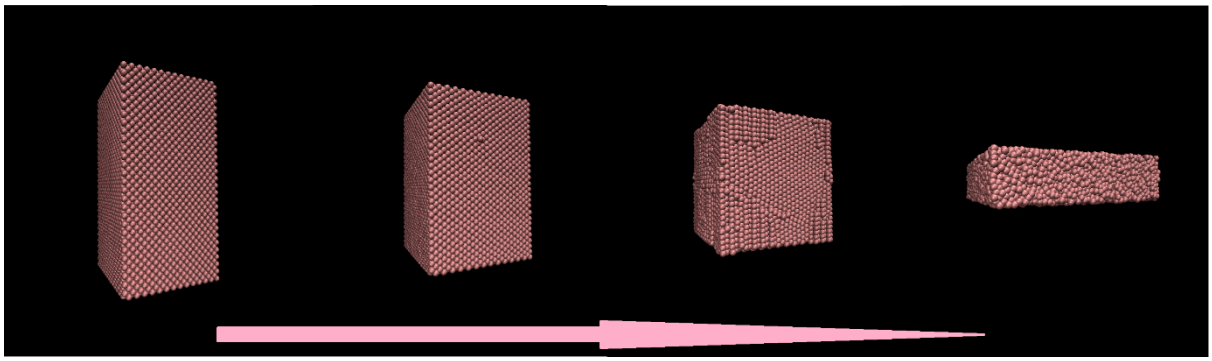


Fig. 3.6.1 VMD snapshot of Compression testing of unnotched specimen during simulation

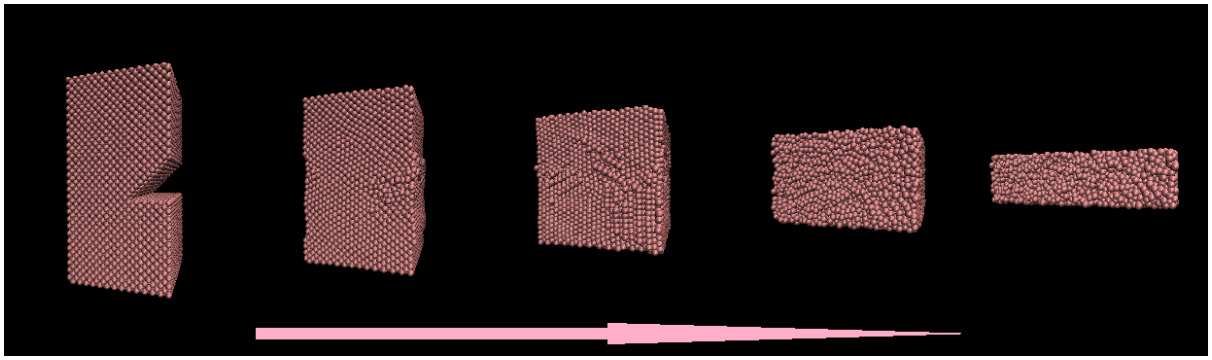


Fig. 3.6.2 VMD snapshot of Compression testing of V-notched specimen during simulation

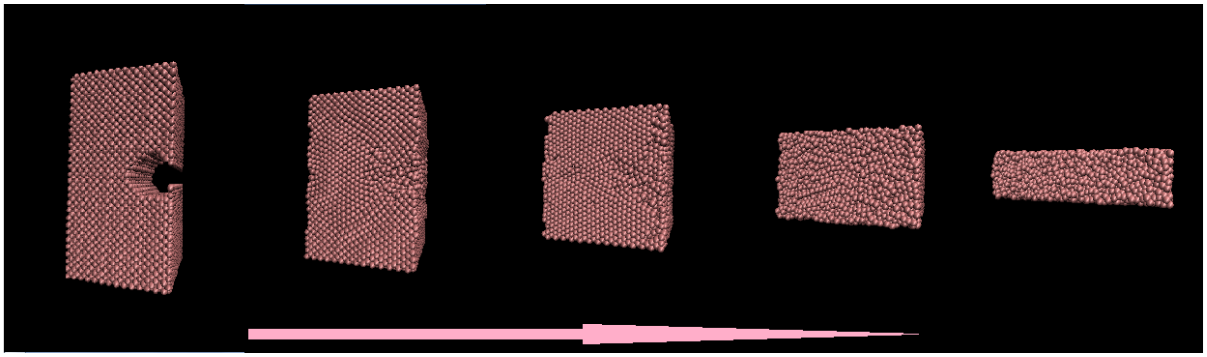


Fig. 3.6.3 VMD snapshot of Compression testing of cylindrical notched specimen during simulation

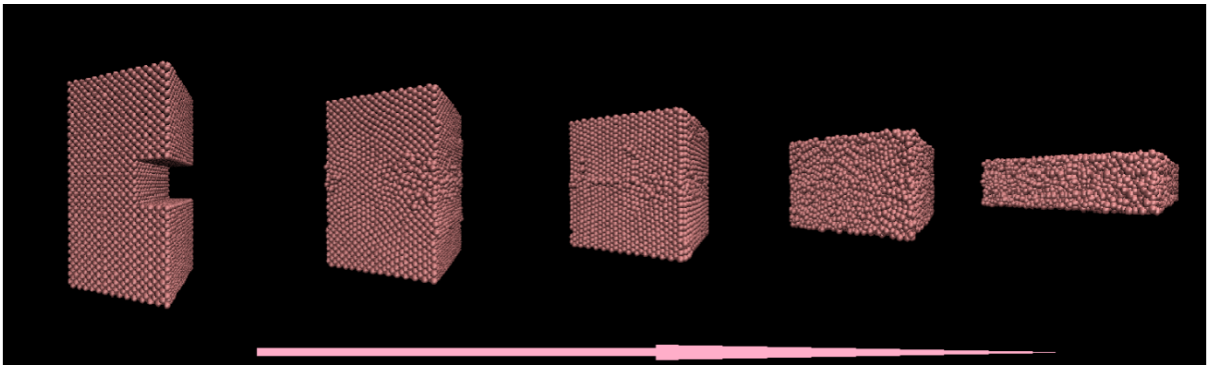


Fig. 3.6.4 VMD snapshot of Compression testing of square notched specimen during simulation

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Results and Discussion

CHAPTER 4

OUTLINE

Tensile properties

(a) Effect of temperature on tensile behaviour

(b) Effect of notch design tensile behaviour

Compression properties

Effect of notch design on compression behavriour

RESULT & DISCUSSION

4.1Tensile Properties:

The primary aim of this investigation is to study the effect of various notch geometries (viz square notched, V- notched, cylindrical notched) on the tensile behaviour of nano-scale pure copper. Before conducting any experiment related to it, Molecular Dynamics simulations using LAMMPS were carried out to find tensile behaviour and hence UTS of the investigated material at various temperatures

4.1.1 Effect of temperature on tensile behaviour

Simulations were carried out at different temperatures to study the effect of temperature on the tensile properties of nano-scale copper of various notch geomrtries. The generated results from tensile simulations were examined and the data were plotted to generate the stress-strain curves of nano-scale copper at various temperatures (100K, 200K 300K,400K and 500K). stress-strain curves are illustrated in the figures below:

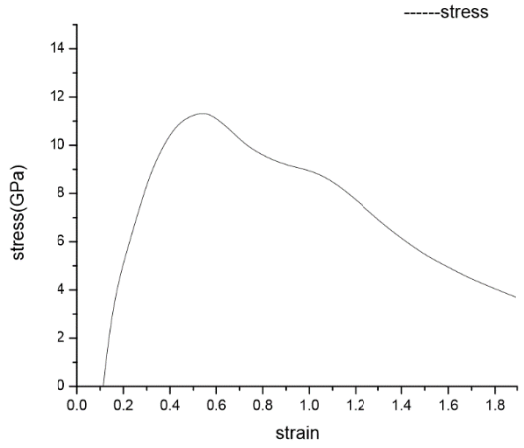

Fig.-4.1 Tensile stress vs strain at 100K in an unnotched specimen

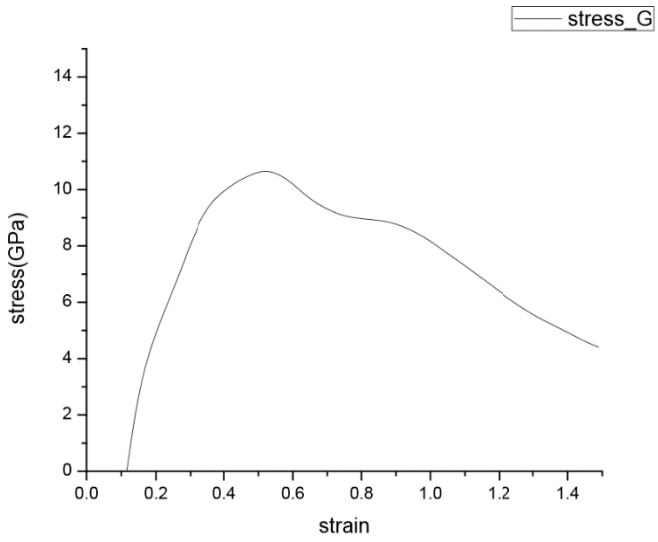

Fig.-4.2Tensile stress vs strain at 200K in a unnotched specimen

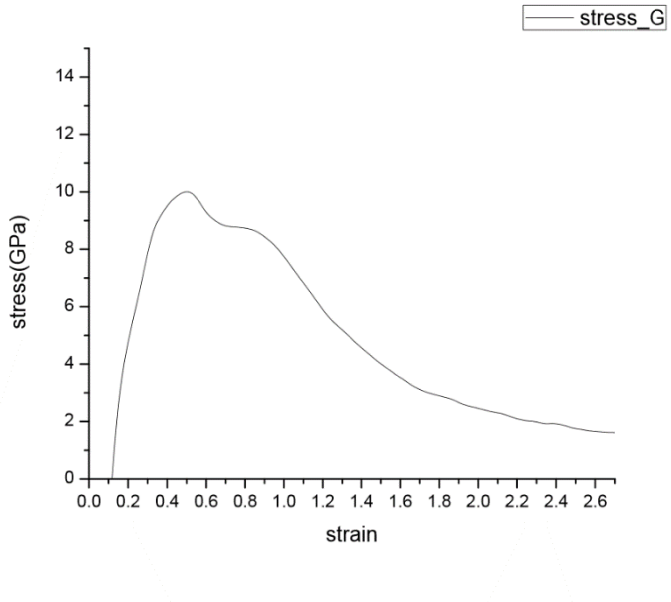

Fig.-4.3 Tensile stress vs strain at 300K in a unnotched specimen

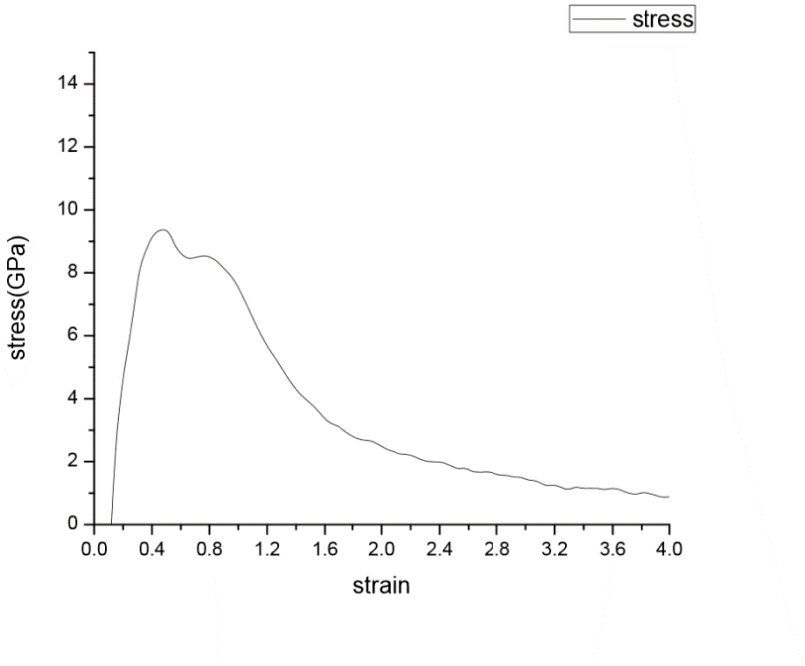

Fig.-4.4 Tensile stress vs strain at 400K in aunnotched specimen

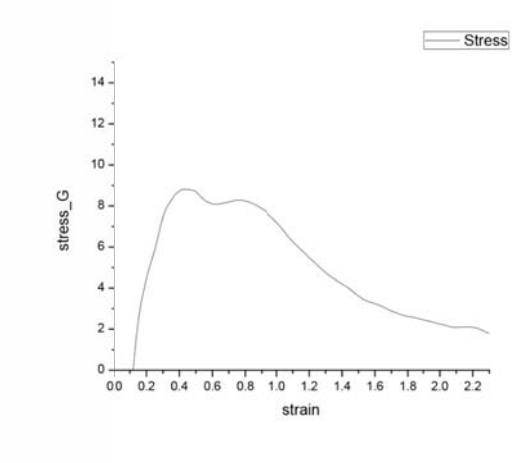

Fig.-4.5 Tensile stress vs strain at 500K in aunnotched specimen

This is well verified that strength of metallic materials decreases with increasing temperature.

From the simulation results on nano-scale copper, similar results has been obtained. The

stress- strain curves at 100 K,200K 300 K ,400Kand 500 K when plotted in a single graph clearly indicate the effect of temperature as illustrated in Fig. 4.6.

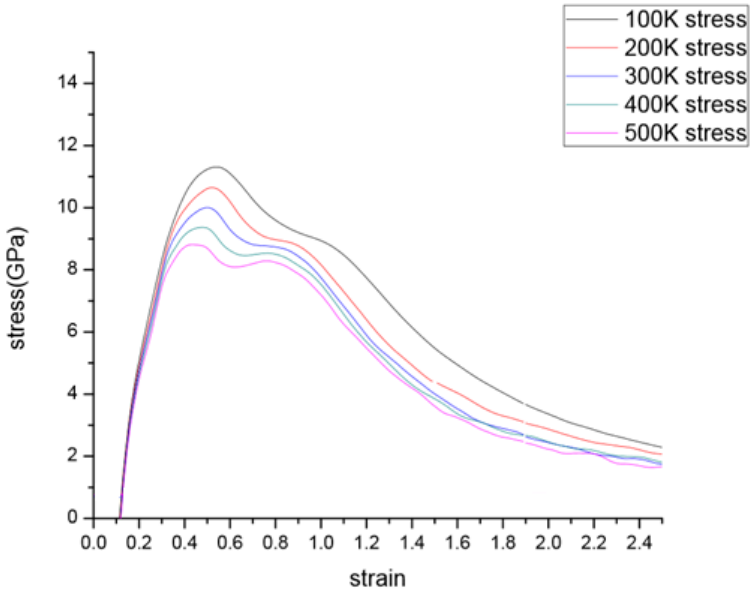

Fig.-4.6 Relationship between Tensile stress vs strain at various temperatures in a unnotched specimen

As the experiment procedure is shown in above, similar procedure is followed for different notch geometries and analysed the effect of temperature on the tensile stress.

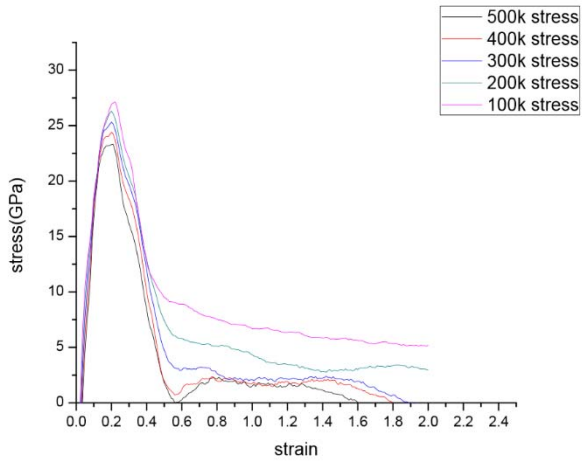

Fig.-4.7 Relationship between Tensile stress vs strain at various temperatures in a square notched specimen

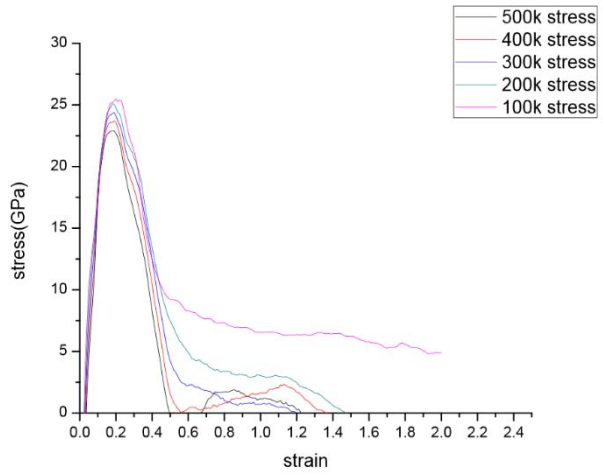

Fig.-4.8 Relationship between Tensile stress vs strain at various temperatures in a cylindrical notched specimen

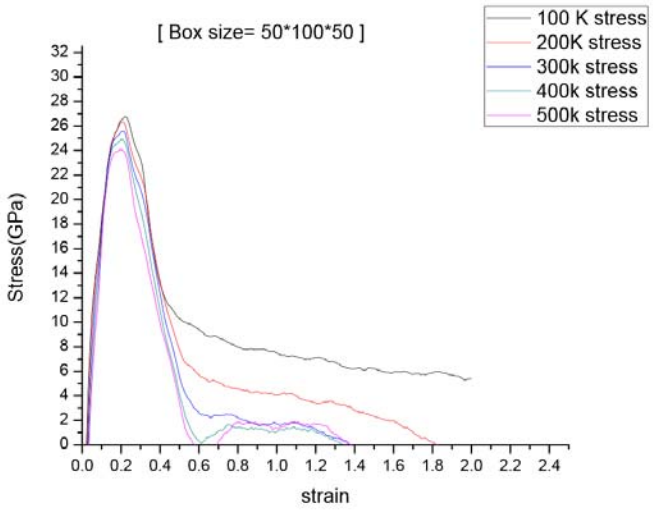

Fig.-4.9 Relationship between Tensile stress vs strain at various temperatures in a V- notched specimen

It can be verified from the figure above that with increase in temperature, the stress-strain curves dropped down, as expected. It is known that flow stress decreases at higher temperatures; similar features can be observed from the current set of simulation studies.

4.1.2. Effect of notch design on tensile behaviour

It can be expected that properties of nano-scale materials should vary based on number of atoms present in a cluster of atoms. This may be interpreted as the variations in notch geometry design. ; Simulations were carried out at different temperatures to study the effect of notch geometry on the tensile properties of nano-scale copper with notch and without notch. The generated results from tensile simulations were examined and the data were plotted to generate the stress-strain curves of nano-scale copper at various notch geometries at a particular temperature and study the effect of different notch geometries on tensile behaviour of nano-scale copper. stress- strain curves are illustrated in the figures below:

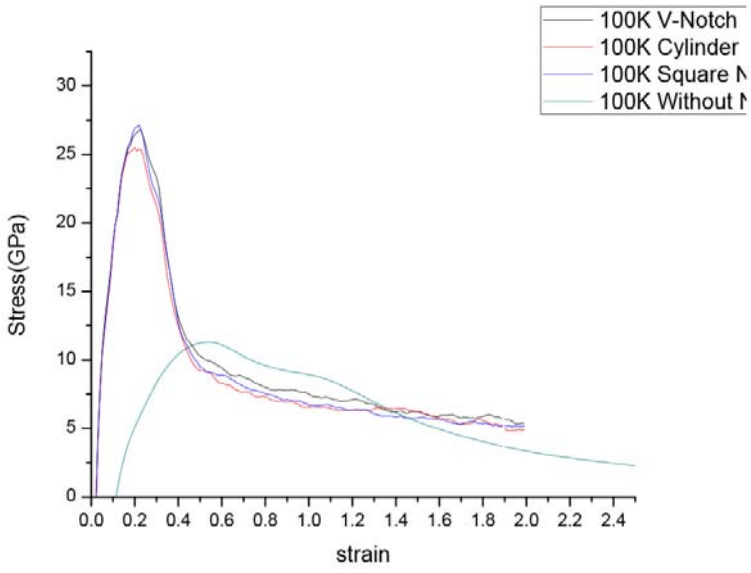

Fig.-4.10 Relationship between Tensile stress vs strain at various notch geometries at 100K

Similarly we can verify the effect of notch geometries on tensile stress at various temperature.

From the fig.-4.10 we can see UTS of un-notched specimen < UTS of cylindrical notched specimen <UTS of prism notched specimen <UTS of square notched specimen

The main effect of the notch is to create stress tri-axiality at the notch.With the introduce of notch it creates a local stress peak at the root of the notch.The tendency for increase tensile strength in presence of a tri-axial stress field is called notch sensitivity.Withthe introduce of notch there comes a plastic constraint factor. Because of this plastic constraint factor tensile strength will be more than an un-notched specimen.

In the following table the value of UTS, YS, % uniform elongation, %total elongation at various notch geometry and at various temperature are calculated from the above stress- strain plot.

Temp.	Material Type.	UTS(GPa)	YS(GPa)	%Uniform elongation	%Total elongation
100K	Without Notch	11.304	4.23	0.552	1.89
100K	Square Notch	27.096	18.89	0.218	1.995
100K	Cylindrical Notch	25.425	24.607	0.212	2.003
100K	V-Notch	26.7	13.09	0.225	2.006
200K	Without Notch	10.614	3.409	0.521	1.49
200K	Square Notch	26.137	17.54	0.197	2.007
200K	Cylindrical Notch	24.906	22.02	0.182	1.47
200K	V-Notch	26.41	13.521	0.205	1.829
300K	Without Notch	9.95	3.99	0.497	2.7
300K	Square Notch	25.117	19.486	0.204	1.89
300K	Cylindrical Notch	24.29	23.22	0.192	1.189
300K	V-Notch	25.627	23.39	0.21	1.381
400K	Without Notch	9.435	5.29	0.461	3.983
400K	Square Notch	24.29	21.43	0.197	1.8
400K	Cylindrical Notch	23.677	22.177	0.191	1.359
400K	V-Notch	24.932	23.53	0.203	1.328
500K	Without Notch	8.806	4.25	0.432	2.3
500K	Square Notch	23.306	21.427	0.212	1.607
500K	Cylindrical Notch	22.927	21.42	0.183	1.219
500K	V-Notch	24.114	22.24	0.2	1.382

4.2 COMPRESSION PROPERTIES

4.2.1.. Effect of notch design on compression behaviour

This may be interpreted as the variations in notch geometry design. ; Simulations were carried out at different temperatures to study the effect of notch geometry on the compression behaviour of nano-scale copper with notched and without notched specimen. The generated results from tensile simulations were examined and the data were plotted to generate the stress-strain curves of nano-scale copper at various notch geometries at a particular temperature and study the effect of different notch geometries on compression behaviour of nano-scale copper. stress- strain curves are illustrated in the figures below

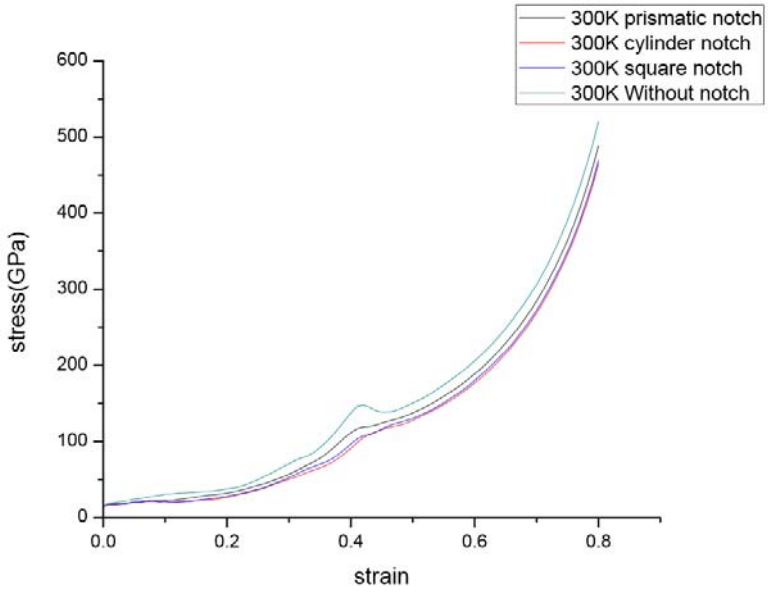

Fig.-4.11 Relationship between compression stress vs strain at various notch geometries at 300K

Similarly we can verify the effect of notch geometries on compression stress at various temperature.

From the fig.-4.11 we can see compression stress of unnotched specimen> compression stress of prism notched specimen> compression stress of square notched specimen>compression stress of cylindrical notched specimen

Conclusions and Future Work Scope

CHAPTER 5

OUTLINE

Conclusions

Future Work scope

5.1 Conclusions:

The influence of temperature and different types of notch geometry on the tensile and compression behaviour of nano-scale copper have been studied using molecular dynamics simulation. According to simulation results, the following conclusions can be derived:

a) The ultimate tensile strength (UTS) of nano-scale copper is found to decrease from 11.304 GPa to 8.806 GPa when temperature varies from 100K to 500K in un-notched condition. Similarly decrease in UTS is found for all notched specimen.

b) It is established that the tensile strength & ductility is greatly dependent on the geometry of the notch. The square notch is having maximum detrimental effect.

c) In a similar manner to the tensile simulations, compression strength of the specimen decreases with the influence of notch geometry. It is found that the cylindrical notch is having maximum detrimental effect..

d) As one can expect the ductility of all notch specimen boxes reduces as compared to that in un-notched conditions. The reduction in ductility occurs due to development of plastic constraint factorin the notched specimens.

MD simulations is a good investigation than those obtained from laboratory experiments. Thus, it can be suggested that MD simulations can predict the tensile and compressionbehaviour of copper.

5.2. Scope of Future work:

In this investigation, tensile and compression behaviour of nano-scale pure copper has been studied. Careful analyses of the outcomes of this investigation may lead to the following scopes of further studies:

(i) To study the prolonged effect of temperature on the compression behaviour of nano-scale copper, simulations on compression can be conducted for various temperatures.

(ii) To study the effect of strain rate and box dimension on tensile behaviour of the materials, simulations on tensile tests can be conducted.

(iii) Similar simulations can be conducted to observe the tensile and compression behaviour of various other FCC materials like nickel, aluminium. The results from these simulations can be used for further analysis and understanding the variation in their tensile and compression behaviour.

(iv) Similar investigation can be done for multiple notches and various notch locations like notches present in end or notches from both sides etc.

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